

## Instructions for Completing the INCITE Proposal Questions

**Note: PDF or Microsoft Word files are acceptable formats for uploaded files.**

### 1. Principal Investigator and Co-Principal Investigators

The Principal Investigator (PI) is primary project contact and responsible managing project and any resources awarded to the project. If your project has multiple investigators, list the Principal Investigator first. Co-PIs can be added one at a time by using the "Add Co-PI" button.

#### **Biographical Sketches**

Provide a 2-page CV for the PI and any Co-PI listed on the proposal. In CV, list all persons, including their current organizational affiliations, who have been collaborators or co-authors with you on a project, book, article, report, abstract or paper within the past 48 months. Also include in the list your graduate and postdoctoral advisors and any graduate students you have advised. This information will be used to help identify potential conflicts or bias in the selection of reviewers.

#### **Institutional Contact**

For the institution of the Principal Investigator, identify the agent who has the authority to review, negotiate, and sign the User Agreement on behalf of that institution. The person who can commit an organization may be someone in the contracts or procurement department, legal, or, if a university, the department head or Sponsored Research Office or Grants Department.

### 2. Project Title

Choose a project title that succinctly describes the project you intend to do.

### 3. Science Category

Select the science category that best categorizes your project. The categories based on the National Science fields of science and engineering found in section 5 at

[http://www.nsf.gov/statistics/nsf07323/content.cfm?pub\\_id=3766&id=3#definitions](http://www.nsf.gov/statistics/nsf07323/content.cfm?pub_id=3766&id=3#definitions)

If none of the categories describe your project, select Other and specify your scientific discipline in the box.

### 4. Project Summary

4.a Please provide a brief one to two paragraph executive summary that accurately describes your proposed research and the high-impact scientific advances you will realize with the proposed INCITE allocation. This section should not exceed one (1) page.

4.b Please provide a project summary in no more than two sentences that could be used to describe the impact of your project to the public.

## 5. Computational Resources Requested

Proposals may request up to three years of resources. However, for successful proposals, allocations in subsequent years are based on an annual project review and will be awarded on only one resource each year.

If your project only needs an allocation on a **single primary** resource, please follow the directions in Section 5.a to identify your primary computing resource. If your project is optimized for running on an alternative system, you may choose one or more alternative resources in Section 5.b. However you must provide evidence that your project is optimized to run on that resource in the Computational Readiness Section (Section 9) of the application.

If your project needs an allocation on **multiple primary** resources, use Section 5.a to identify a set of **primary** resources for each year. Similarly, if your project is optimized for running on **alternative** resources, if needed, use Section 5.b to select a set of **alternative** resources for each year. You must clearly justify the need for allocations of multiple resources in the Description of Research (Section 8) and in the Computational Readiness (Section 9) sections of the application.

Once you have selected the year and identified a computational resource press ADD Resource and then state your needs for processor hours, storage, and any off-line storage.

### Processor hours :

This is total connect (or wall clock) time multiplied by the number of processors used or in the case of NERSC use MPP hours as explained at <http://www.nersc.gov/nusers/accounts/charging/>

### Gigabytes of storage:

State your needs for both home directory storage and scratch storage.

### Gigabytes or terabytes of mass storage:

State your archival storage requirements.

## 6. Funding Sources

6.a List the Program Office and grant numbers for any Department of Energy's Office of Science support of the project (Note: INCITE projects are not required to be DOE grant supported)

6.b If applicable, list any other funding sources together with the applicable grant number

that support this project.

## **7. Other High Performance Computing Support for this Project**

List any other high performance computing allocations being received from outside the Office of Science in support of this project.

## **8. Description of Research**

### **8.a Research Objectives**

Describe the proposed research, including its goals, milestones and the theoretical and computational methods it employs. This section, including references, should not exceed six (6) pages. Proposals will be evaluated on both scientific and computational merit, so the information should be sufficient for peer review in your area of research and also appropriate for general scientific review comparing your proposal with proposals in other disciplines.

### **8.b Significance of Research**

Place the proposed research in the context of competing work in your discipline. In addition, explain what scientific advance you expect to be enabled by an INCITE award that justifies an urgent allocation of large-scale resources. This section, including any references you provide should not exceed four (4) pages.

## **9. Computational Readiness**

### **9.a Application Packages.**

List each application or software package to be used in the project, including analysis packages and indicate if the software is open source or export controlled. If export controlled, list the export control classification number.

### **9.b Computational Approach**

For the primary and any alternative computational resource selected in section 5. provide the following information:

- Programming languages, libraries, and other software used.
- Description of the underlying mathematical formulation (e.g., ODE, PDE)
- Algorithms and numerical techniques employed (e.g., finite element, iterative solver).
- Parallel programming system used (e.g., MPI, OpenMP, embarrassingly parallel).
- Description of the role collaborative analysis/visualization plays in the discovery process; identify any current bottlenecks in the analysis process.

This section, including any references you provide should not exceed four (4) pages.

### 9.c Job Characterization

- Description of processor/core utilization for large runs (e.g. 10,000 hour run with 100 cores, or ten 10 hour runs with 10,000 cores, for a 1,000,000 hour allocation).
- Explain how you calculated the requested number of processor hours
- Estimate the percentage of project time you will spend on development (porting, code analysis, performance improvement) production computing and other.

### 9.d Application Parallel Performance

Provide direct evidence, including *supporting quantitative data*, for the parallel performance of your application. Parallel performance data in either strong or weak scaling mode *must* be provided. Weak scaling behaviors are probed by holding per-node computational work constant (e.g., the size of the mesh on a processor is held constant) as the total problem size grows with processor count. Strong scaling behaviors are probed by holding the total problem size constant as the processor count grows, thereby decreasing the per-processor computational work. Supporting quantitative data should be provided in either tabular or graphical form, or both; also a speedup curve should be supplied for strong scaling examples. Also, where appropriate, characterize the single-node performance of the application (e.g. percent of peak).

If the performance data indicates less than 50% efficiency on less than 256 nodes, please delineate the path forward for achieving greater performance on much larger scale simulations with the requested INCITE resources. Without this data, application readiness cannot be adequately ascertained and hence awarding this INCITE allocation request will be placed in jeopardy.

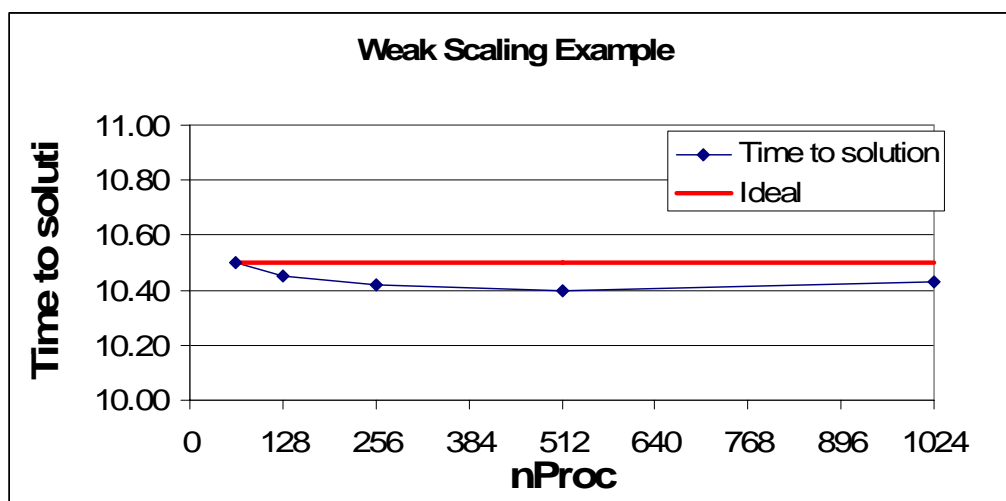
**NOTE: If the supporting quantitative data is not available for your application, you may apply for a start-up account at one of the centers to conduct performance studies. Applications for start-up accounts are available at**

ANL <http://www.bgl.mcs.anl.gov/>  
 LBNL <http://www.nersc.gov/nusers/accounts/allocations/ercap/firsttime.php>  
 ORNL [https://secure.ccs.ornl.gov/new\\_request.html](https://secure.ccs.ornl.gov/new_request.html)  
 PNL <http://mscf.emsl.pnl.gov/accounts/>

An example of the kind of parallel performance data sought is given in the following examples.

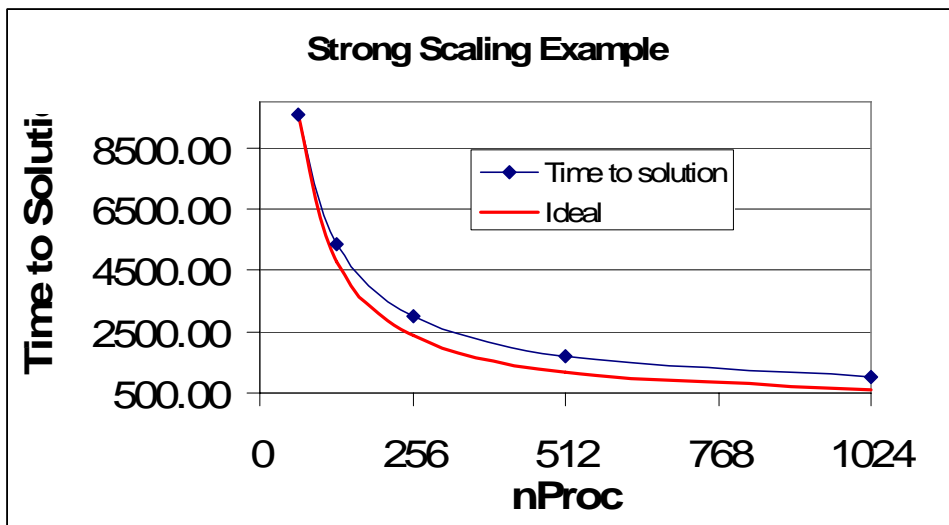
#### Weak Scaling Example

nProc	Time to solution	Ideal
64	10.50	10.50
128	10.45	10.50
256	10.42	10.50
512	10.40	10.50
1024	10.43	10.50



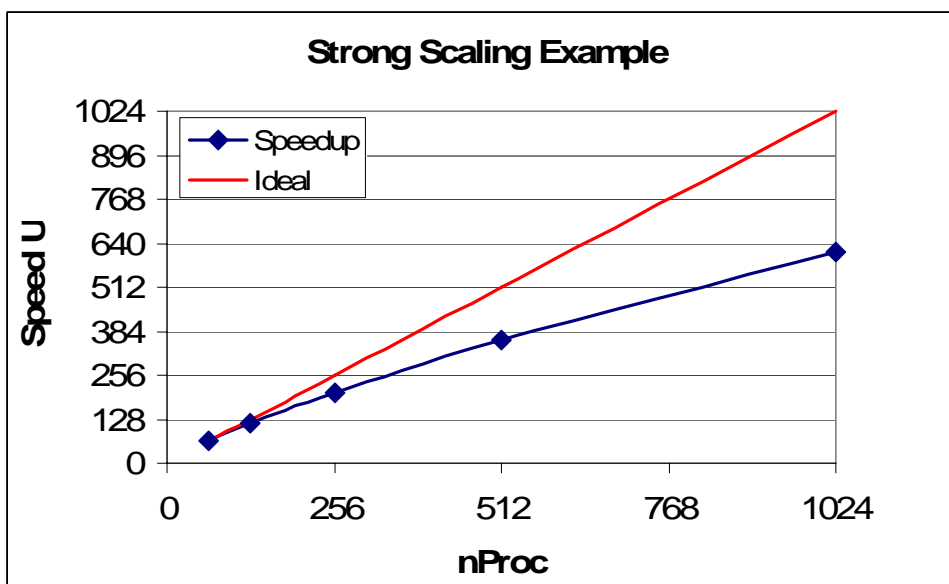
#### Strong Scaling Example

nProc	Time to solution	Ideal
64	9600.00	9600.00
128	5333.33	4800.00
256	3000.00	2400.00
512	1714.29	1200.00
1024	1000.00	600.00



### Strong Scaling Example

nProc	Speedup	Ideal
64	64.00	64.00
128	115.20	128.00
256	204.80	256.00
512	358.40	512.00
1024	614.40	1024.00



## 9.e I/O Requirements

**Restart I/O.** Describe I/O requirements for program restart. Include a list of the file types written out for program restarts such as MPI/IO, raw binary, serial from all processors, HDF5, etc. and the following quantitative information: amount of restart data written out, number of processors writing out restart data, amount of memory job takes per processor, the size of a single restart dump and acceptable time to read/write restart data.

**Analysis I/O.** Describe I/O requirements for analysis, including types of files written out for analysis such as HDF5, NetCDF, PHDF5, PnedtCDF; size of analysis dump, amount and type of data read into analysis program.

**Data Transfer I/O.** Describe your external data access requirements. Include details on the following: your bandwidth requirements, the average and maximum size of data transfers and the frequency of data transfers.

**Archival I/O.** Describe your archival data requirements. Include details on the following: total space needed; file size distribution (many small files or one large file), access pattern, retention needs and frequency of access.

## 10. Proprietary and Sensitive Information

Principal Investigators are responsible for knowing whether their project uses or generates proprietary, sensitive or restricted information.

### 10.a Does this project use or generate proprietary information?

Select **Yes** or **No**.

Proprietary use of the HPC resources by industry is subject to the successful completion of negotiation with the Department of Energy of the Terms and Conditions including cost recovery and approval of the Department of Energy General Counsel.

### 10.b Does this project use or generate sensitive or restricted information?

Select **Yes** or **No**.

Principal Investigators are responsible for knowing whether their project uses or generates sensitive or restricted information. Dept. of Energy systems contain data only related to scientific research and do not contain personally identifiable information. Therefore, you should answer **Yes** if your project uses or generates data that falls under the Privacy Act of 1974 U.S.C. 552a. Use of High Performance Computing resources to

store, manipulate, or remotely access any national security information is prohibited. This includes, but is not limited to, classified information, unclassified controlled nuclear information (UCNI), naval nuclear propulsion information (NNPI), the design or development of nuclear, biological, or chemical weapons or of any weapons of mass destruction. For more information contact the Office of Domestic and International Energy Policy, Department of Energy, Washington DC 20585 , 202-586-9211.

## **11. Export Control**

The following questions are provided to determine whether research associated with an INCITE proposal may be export controlled. Responding to these questions can facilitate, not substitute, for any export control review required by the selected site.

### **11. Select Yes or No**

- Does the proposed project involve any of the following areas? Military, Space Craft, Satellites, Missiles, and associated hardware, software or technical data; Nuclear Reactors & Components, Nuclear Material Enrichment Equipment, Components (Trigger List) and associated hardware, software or technical data; Encryption above 128 bit software (source & object code); Weapons of Mass Destruction or their precursors (nuclear, chemical & biological)
- Does the proposed project use and/or create proprietary information, intellectual property, licensing, or will utilize information in any of these categories in pursuit of the project objectives?
- Are the proposed project and its intended subject matter deliverables considered Fundamental Research or Publicly Available Information as under National Security Decision Directive - 189?

NSDD 189 defines Fundamental Research as "basic and applied research in science and engineering, the results of which ordinarily are published and shared broadly within the scientific community, as distinguished from proprietary research and from industrial development, design, production, and product utilization, the results of which ordinarily are restricted for proprietary or national security reasons." Publicly Available Information is defined as information obtainable free of charge (other than minor shipping or copying fees) and without restriction; which is available via the internet, journal publications, text books, articles, newspapers, magazines, etc.

## **12. Monitor Information**

### **Check box.**

Department of Energy Principal Investigators and their designated Project Managers are responsible for monitoring the computer usage associated with their project and ensuring compliance with all U.S. Export Controls.